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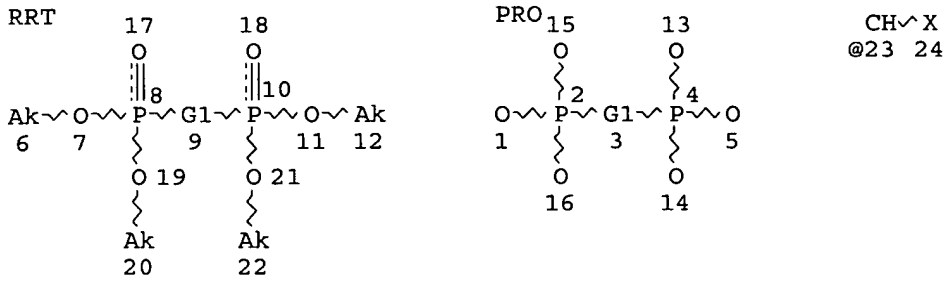

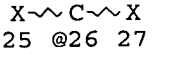


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CONNECT IS E1  RC AT   5
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CONNECT IS E1  RC AT  16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS  27

STEREO ATTRIBUTES: NONE
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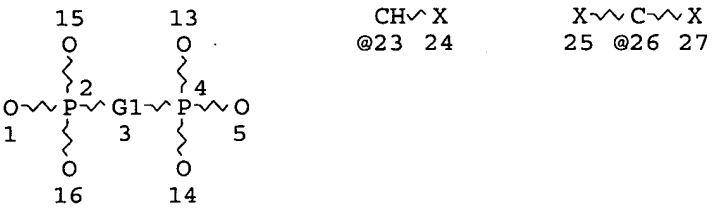


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VAR G1=CH2/23/26
NODE ATTRIBUTES:
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CONNECT IS E1  RC AT   5
CONNECT IS E1  RC AT  13
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CONNECT IS E1  RC AT  15
CONNECT IS E1  RC AT  16
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
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STEREO ATTRIBUTES: NONE
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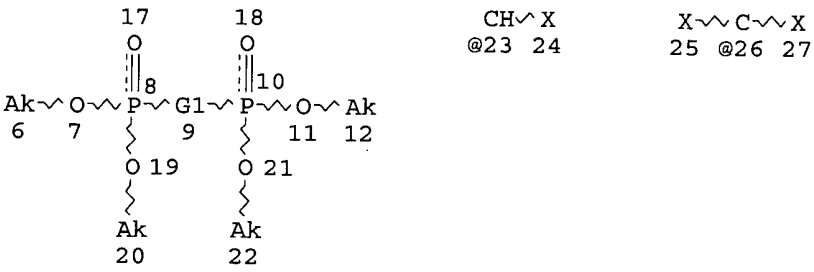

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DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED

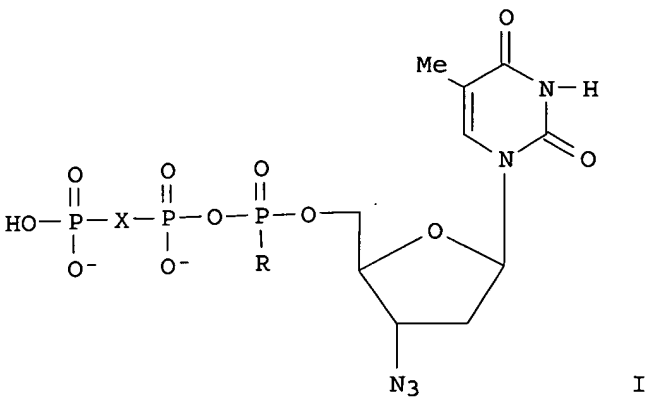
GRAPH ATTRIBUTES:
RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 18

STEREO ATTRIBUTES: NONE
L9 229 SEA FILE=REGISTRY SSS FUL L7
L10 38 SEA FILE=HCAPLUS ABB=ON PLU=ON L9(L)(RACT OR RGT OR RCT)/RL AND L6(L)PREP/RL
L11 1 SEA FILE=REGISTRY ABB=ON PLU=ON N-BUTANOL/CN
L12 2596 SEA FILE=REGISTRY ABB=ON PLU=ON 71-36-3/CRN OR L11
L13 1 SEA FILE=REGISTRY ABB=ON PLU=ON "HYDROCHLORIC ACID"/CN
L14 138 SEA FILE=REGISTRY ABB=ON PLU=ON 7647-01-0/CRN OR L13
L15 2 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 AND (L12 OR L14)
L16 38 SEA FILE=HCAPLUS ABB=ON PLU=ON L10 OR L15
L17 28 SEA FILE=HCAPLUS ABB=ON PLU=ON L16 NOT L3

=> d l17 ibib abs hitstr 1-28

L17 ANSWER 1 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2004:1048934 HCAPLUS
DOCUMENT NUMBER: 142:198289
TITLE: Synthesis of AZT 5'-Triphosphate Mimics and Their Inhibitory Effects on HIV-1 Reverse Transcriptase
AUTHOR(S): Wang, Guangyi; Boyle, Nicholas; Chen, Fu; Rajappan, Vasanthakumar; Fagan, Patrick; Brooks, Jennifer L.; Hurd, Tiffany; Leeds, Janet M.; Rajwanshi, Vivek K.; Jin, Yi; Prhavc, Marija; Bruice, Thomas W.; Cook, P. Dan
CORPORATE SOURCE: Research Laboratories, Biota, Inc., Carlsbad, CA, 92008, USA
SOURCE: Journal of Medicinal Chemistry (2004), 47(27), 6902-6913
CODEN: JMCMAR; ISSN: 0022-2623
PUBLISHER: American Chemical Society
DOCUMENT TYPE: Journal
LANGUAGE: English

GI



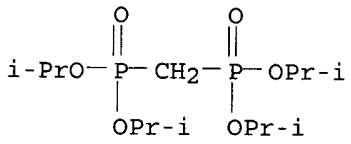
I

AB In search of active nucleoside 5'-triphosphate mimics, we have synthesized a series of AZT triphosphate mimics (AZT P3Ms) and evaluated their inhibitory effects on HIV-1 reverse transcriptase as well as their stability in fetal calf serum and in CEM cell exts. Reaction of AZT with 2-chloro-4H-1,3,2-benzodioxaphosphorin-4-one, followed by treatment of the phosphite intermediate with pyrophosphate analogs, yielded the cyclic triphosphate intermediates, which were subjected to boronation and subsequent hydrolysis to give AZT 5'-α-borano-β,γ-bridge-modified triphosphates, e.g. I (X = O, R = -BH3; X = CF2, R = O-), in moderate to good yields. Several different types of AZT P3Ms containing α-P-thio (or dithio) and β,γ-difluoromethylene, α,β-difluoromethylene and γ-P-methyl(or phenyl), and α-borano-β,γ-difluoromethylene and γ-O-methyl/phenyl were also synthesized. The effectiveness of the compds. as inhibitors of HIV-1 reverse transcriptase was determined using a fluorometric assay and a poly(A) homopolymer as a template. A number of title compds. exhibited very potent inhibition of HIV-1 reverse transcriptase. Modifications at the β,γ-bridge of triphosphate rendered the AZT P3Ms 6b-6f with varied activities (Ki from 9.5 to » 500 nM) while modification at the α,β-bridge of triphosphate led to weak AZT P3M inhibitors. The results imply that the AZT P3Ms were substrate inhibitors, as is AZT triphosphate. The most active compound, AZT 5'-α-Rp-borano-β,γ-(difluoromethylene)triphosphate (AZT 5'-αB-βγCF2TP) (6d-I), is as potent as AZT triphosphate with a Ki value of 9.5 nM and at least 20-fold more stable than AZT triphosphate in the serum and cell exts. Therefore, for the first time, a highly active and stable nucleoside triphosphate mimic has been identified, which is potentially useful as a new type of antiviral drug. The promising triphosphate mimic, 5'-α-borano-β,γ-(difluoromethylene)triphosphate, is expected to be valuable to the discovery of nucleotide mimic antiviral drugs.

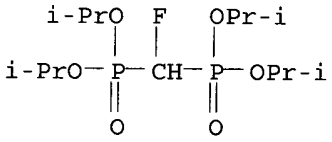
IT **1660-95-3**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(synthesis of AZT triphosphate mimics and their inhibitory effects on HIV reverse transcriptase)

RN 1660-95-3 HCAPLUS

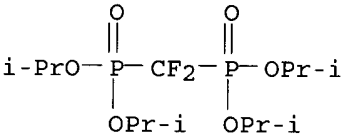
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **78715-57-8P 78715-59-0P 81336-71-2P**
92340-84-6P 104714-96-7P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(synthesis of AZT triphosphate mimics and their inhibitory effects on HIV reverse transcriptase)
RN 78715-57-8 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



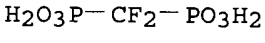
RN 78715-59-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 81336-71-2 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

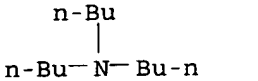
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2



CM 2

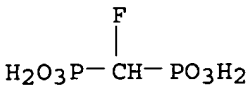
CRN 102-82-9
CMF C12 H27 N



RN 92340-84-6 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

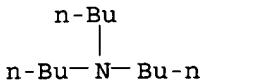
CM 1

CRN 10595-93-4
CMF C H5 F O6 P2



CM 2

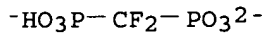
CRN 102-82-9
CMF C12 H27 N



RN 104714-96-7 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, (difluoromethylene)bis[phosphonate] (3:1) (9CI) (CA INDEX NAME)

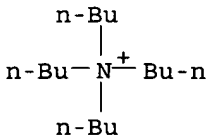
CM 1

CRN 104714-95-6
CMF C H F2 O6 P2



CM 2

CRN 10549-76-5
CMF C16 H36 N



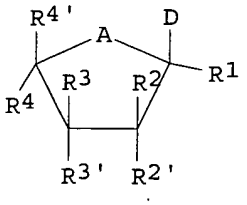
REFERENCE COUNT: 35 THERE ARE 35 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2003:697043 HCAPLUS
DOCUMENT NUMBER: 139:230954
TITLE: Preparation of nucleotide mimics and their prodrugs as antiviral, antibacterial, and antitumor agents
INVENTOR(S): Cook, Phillip Dan; Wang, Guangyi; Bruice, Thomas W.; Boyle, Nicholas A.; Leeds, Janet M.; Brooks, Jennifer L.; Prhavc, Marija; Ariza, Maria Eugenia; Fagan, Patrick C.; Jin, Yi; Rajwanshi, Vivek K.; Tucker, Kathleen D.
PATENT ASSIGNEE(S): Biota, Inc., USA
SOURCE: PCT Int. Appl., 184 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2003072757	A2	20030904	WO 2003-US6368	20030228
WO 2003072757	A3	20040722		
WO 2003072757	C2	20041021		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
CA 2477741	AA	20030904	CA 2003-2477741	20030228
US 2004059104	A1	20040325	US 2003-376654	20030228
EP 1485395	A2	20041215	EP 2003-713832	20030228
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				

PRIORITY APPLN. INFO.:
US 2002-360699P P 20020228
US 2002-360915P P 20020228
WO 2003-US6368 W 20030228

OTHER SOURCE(S): MARPAT 139:230954
GI

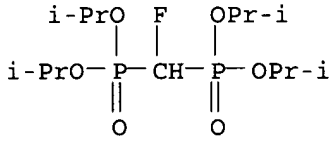


I

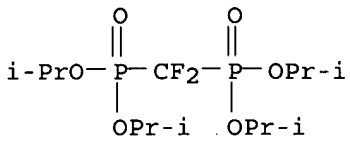
AB Nucleotide diphosphate mimics and nucleotide triphosphate mimics I, wherein A is O, S, NH, NR; R4' is LR5; L is O, S, NH, NR, CY2O, CY3S, CY2NH, CY2, CY2CY2, CY2OCY2, CY2SCY2, CY2NHCY2; Y is H, halogen, alkyl, alkenyl, alkynyl, R5 is substituted di- or triphosphate; R is alkyl, alkenyl, alkynyl, aryl, acyl, aralkyl; R1-R4 and R2'-R3' are independently H, halogen, OH, SH, NH2, NHOH, N3, NO2, CHO, CO2H, CN, CONH2, CO2R, R, OR, SR, SSR, NHR, NR2; D is nucleobase, which contain diphosphate or triphosphate moiety mimics and optionally sugar-modifications and/or base-modifications were prepared as antiviral, antibacterial, and antitumor agents. The present invention provides a method for the treatment of viral infections, microbial infections, and proliferative disorders. The present invention also relates to pharmaceutical compns. comprising the compds. of the present invention optionally in combination with other pharmaceutically active agents. Thus, 3'-azido-3'-deoxythymidine 5'-α-P-borano-β,γ-(difluoromethylene)triphosphate was prepared and tested in vitro as antiviral, antibacterial, and antitumor agent and HIV reverse transcriptase inhibitor (Ki = 0.008-0.061 μM).

IT **78715-57-8P 78715-59-0P 81336-70-1P 81336-71-2P 92340-84-6P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation of nucleotide mimics and their prodrugs as antiviral antibacterial and antitumor agents)

RN 78715-57-8 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



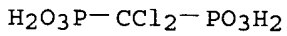
RN 78715-59-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 81336-70-1 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

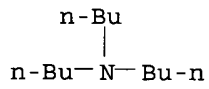
CM 1

CRN 10596-23-3
CMF C H4 Cl2 O6 P2



CM 2

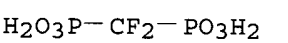
CRN 102-82-9
CMF C12 H27 N



RN 81336-71-2 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

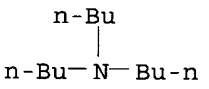
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2



CM 2

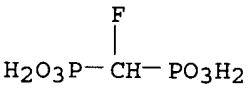
CRN 102-82-9
CMF C12 H27 N



RN 92340-84-6 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:2) (9CI) (CA INDEX NAME)

CM 1

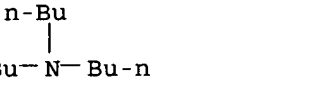
CRN 10595-93-4
CMF C H5 F O6 P2



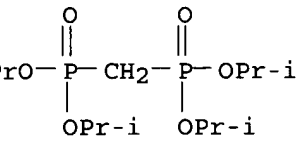
CM 2

CRN 102-82-9

CMF C12 H27 N



IT **1660-95-3**
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(preparation of nucleotide mimics and their prodrugs as antiviral antibacterial and antitumor agents)
RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



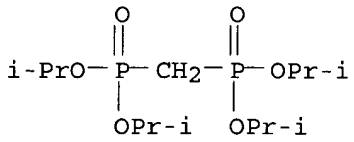
L17 ANSWER 3 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2002:125501 HCAPLUS
DOCUMENT NUMBER: 136:134917
TITLE: Method for preparation of methylene diphosphonic acid
INVENTOR(S): Cho, Jeong Hyeok; Oh, Chang Hyeon; Lee, Ki Su; Lee, Chang Sik; Lee, Myeong Cheol; Jeong, Jun Ki; Lee, Dong Su; Jeong, Jae Min
PATENT ASSIGNEE(S): Korea Institute of Science and Technology, S. Korea
SOURCE: Repub. Korean Kongkae Taeho Kongbo, No pp. given
CODEN: KRXXA7
DOCUMENT TYPE: Patent
LANGUAGE: Korean
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
KR 2000020033	A	20000415	KR 1998-38443	19980917
PRIORITY APPLN. INFO.:			KR 1998-38443	19980917

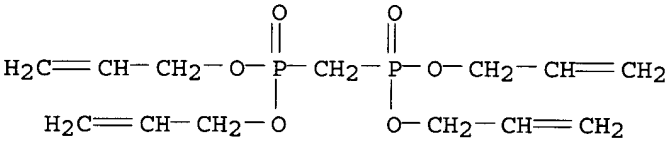
AB A preparation method of methylene diphosphonic acid (I) by using diidomethane having a higher b.p. than reaction temperature is provided which produces the title compound I in high yield, improves high productivity and is very economic by reusing trialkyl phosphate as a starting material. A process is disclosed for preparing I which comprises: (a) preparing methylenediphosphonic acid tetraalkyl ester (II; wherein the alkyl is allyl, iso-Pr, t-Bu, or iso-Bu) by reacting trialkyl phosphate with diiodomethane; (b) separating the compound II from the reactant by removing alkyl iodine; (c) recovering excess trialkyl phosphate by distillation at 180° and recycling to the process (a); (d) removing alkyl groups by thermal-cracking the ester at 200-210° and recrystg. The compound is useful as raw material for radioactive pharmaceuticals for diagnosis.
IT **1660-95-3P**, Methylenediphosphonic acid tetraisopropyl ester
25091-05-8P 64630-15-5P, Methylenediphosphonic acid

tetra-isobutyl ester **393589-31-6P**
RL: IMF (Industrial manufacture); **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(method for preparation of methylenediphosphonic acid by alkylation trialkyl phosphate with diiodomethane and deesterification (thermal cracking) of methylenediphosphonic acid tetraalkyl ester)

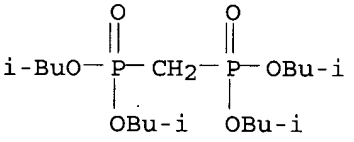
RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



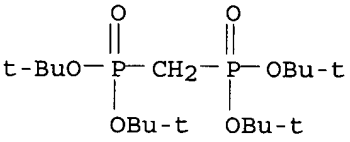
RN 25091-05-8 HCAPLUS
CN Phosphonic acid, methylenebis-, tetra-2-propenyl ester (9CI) (CA INDEX NAME)



RN 64630-15-5 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(2-methylpropyl) ester (9CI) (CA INDEX NAME)

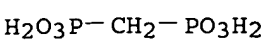


RN 393589-31-6 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1,1-dimethylethyl) ester (9CI) (CA INDEX NAME)



IT **1984-15-2P**, Methylenediphosphonic acid
RL: IMF (Industrial manufacture); SPN (Synthetic preparation); **PREP (Preparation)**
(method for preparation of methylenediphosphonic acid by alkylation trialkyl phosphate with diiodomethane and deesterification (thermal cracking) of

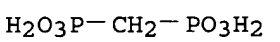
methylenediphosphonic acid tetraalkyl ester)
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)



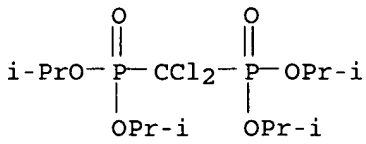
L17 ANSWER 4 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:610709 HCAPLUS
DOCUMENT NUMBER: 133:164172
TITLE: Preparation of methylenediphosphonic acid
INVENTOR(S): Marazza, Fabrizio
PATENT ASSIGNEE(S): Cerbios-Pharma S.A., Switz.
SOURCE: Patentschrift (Switz.), 4 pp.
CODEN: SWXXAS
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
CH 690103	A	20000428	CH 1996-3038	19961211
PRIORITY APPLN. INFO.:			CH 1996-3038	19961211

AB The preparation of title compound is described. Thus, reaction of tetraisopropyl
dichloromethylenediphosphonate with C3-6 alc. followed by refluxing the solution at 90-120° for 6-48 h. gave title compound, methylenediphosphonic acid.
IT **1984-15-2P**, Methylenediphosphonic acid
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)

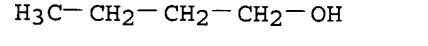


IT **10596-22-2**, Tetraisopropyl dichloromethylenediphosphonate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction with Bu alc.)
RN 10596-22-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)

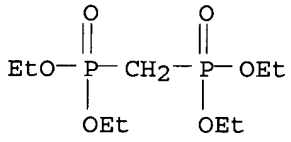


IT **71-36-3**, Butyl alcohol, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(reaction with tetraisopropyl dichloromethylenediphosphonate)

RN 71-36-3 HCAPLUS
CN 1-Butanol (9CI) (CA INDEX NAME)



L17 ANSWER 5 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 2000:443677 HCAPLUS
DOCUMENT NUMBER: 133:171382
TITLE: Synthesis and comparative study of the chelating properties of methylenediphosphonic acid derivatives
AUTHOR(S): Etienne, M.; Rubini, P.; Bessiere, J.; Walcarius, A.; Grison, C.; Coutrot, Ph.
CORPORATE SOURCE: Laboratoire de Chimie Physique pour l'Environnement, UMR 7564 CNRS, Universite Henri Poincare, Vandoeuvre-les-Nancy, 54506, Fr.
SOURCE: Phosphorus, Sulfur and Silicon and the Related Elements (2000), 161, 75-96
CODEN: PSSLEC; ISSN: 1042-6507
PUBLISHER: Gordon & Breach Science Publishers
DOCUMENT TYPE: Journal
LANGUAGE: French
AB Two acid derivs. of methylenediphosphonic acid (MDP) with two inequivalent P atoms were synthesized: [(thiophosphonato)methyl]phosphonic acid, [(HO)2P(S)CH2P(O)(OH)2, MDPS], and [(isopropylamidophosphonato)methyl]phosphonic acid, [(HO)2P(O)CH2P(O)(OH)NHiPr, MDPN]. A potentiometric study was performed to define the stoichiometry of the complex formed between MDP and Mg(II) in alkaline medium and a 31P NMR study proved the dissym. structure of this MDP-Mg(II) complex. The displacement of the coordination equilibrium between Black Eriochrome T and Mg(II) allowed comparison of the coordination strength of MDP, MDPS and MDPN with the cation Mg2+.
IT **1660-94-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and O-silylation of)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



IT **1984-15-2P**, Methylenediphosphonic acid
RL: PRP (Properties); RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation, protonation consts., and complexation with magnesium(II))
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)

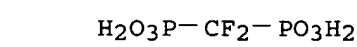
REFERENCE COUNT: 39 THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 6 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1999:235958 HCAPLUS
DOCUMENT NUMBER: 131:19227
TITLE: New modified nucleoside 5'-triphosphates: synthesis, properties towards DNA polymerases, stability in blood serum and antiviral activity
AUTHOR(S): Shipitsin, Alexander V.; Victorova, Lyubov S.; Shirokova, Elena A.; Dyatkina, Natalya B.; Goryunova, Lyudmila E.; Beabealashvilli, Robert Sh.; Hamilton, Chris J.; Roberts, Stanley M.; Krayevsky, Alexander
CORPORATE SOURCE: Engelhardt Institute of Molecular Biology, Russian Academy of Sciences, Moscow, 117984, Russia
SOURCE: Journal of the Chemical Society, Perkin Transactions 1: Organic and Bio-Organic Chemistry (1999), (8), 1039-1050
CODEN: JCPRB4; ISSN: 0300-922X
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

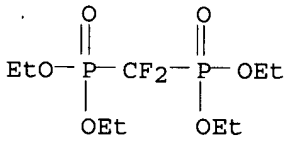
AB A series of new nucleoside 5'-triphosphate mimetics, modified at the aglycon and all three phosphate residues, have been synthesized and studied. These compds. only bear the enzymically labile anhydride bond between the α and β phosphorus atoms. The mechanism of formation of some of the intermediates is discussed. All of the target compds. demonstrated high stability in human blood serum with half lives towards hydrolysis of up to 4.5 days. Some of these nucleoside triphosphonates have been shown to be selective inhibitors of DNA synthesis catalyzed by retroviral reverse transcriptases and terminal deoxynucleotidyl transferases. They inhibited replication of the artificial virus containing Moloney murine leukemia virus reverse transcriptase in infected cell culture, probably due to the inhibition of a reverse transcription step of a genomic RNA. Compared to the triphosphonates, the corresponding monophosphonates demonstrated decreased antiviral activity by 1-2 orders of magnitude. This implies that the triphosphonates inhibit virus replication directly, rather than by a two-step mechanism based on their hydrolysis to the monophosphonates and subsequent intracellular diphosphorylation. Being totally independent of the enzymic phosphorylation pathways of the host cell, the compds. under study may also be able to inhibit retrovirus reproduction both in kinase deficient cell lines and in the intercellular blood media.

IT **10596-32-4P 78715-58-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(synthesis and properties of nucleoside triphosphates towards DNA polymerases stability in blood serum and antiviral activity)

RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)



RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



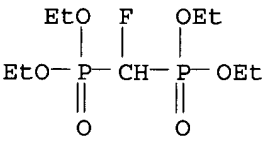
REFERENCE COUNT: 47 THERE ARE 47 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 7 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:342111 HCAPLUS
DOCUMENT NUMBER: 129:81908
TITLE: Synthesis of a potent inhibitor of HIV reverse transcriptase
AUTHOR(S): Hamilton, Chris J.; Roberts, Stanley M.; Shipitsin, Alexander
CORPORATE SOURCE: Department of Chemistry, Exeter University, Exeter, Devon, EX4 4QD, UK
SOURCE: Chemical Communications (Cambridge) (1998), (10), 1087-1088
CODEN: CHCOFS; ISSN: 1359-7345
PUBLISHER: Royal Society of Chemistry
DOCUMENT TYPE: Journal
LANGUAGE: English

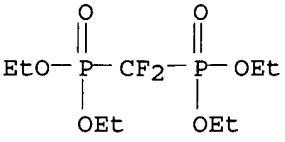
AB The newly synthesized Pβ,-Pγ-difluoromethylenebisphosphonate analog of nor-carbovir triphosphate is a potent inhibitor of HIV reverse transcriptase; it also exhibits a greatly enhanced stability to dephosphorylation, in fetal blood serum, relative to AZTTP and other nucleoside triphosphates.

IT **78715-56-7P 78715-58-9P 139302-00-4P 209454-90-0P 209454-91-1P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(preparation of a potent inhibitor of HIV reverse transcriptase)

RN 78715-56-7 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



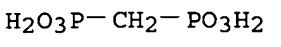
RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



RN 139302-00-4 HCAPLUS
CN Phosphonic acid, methylenebis-, compd. with N,N-dibutyl-1-butanamine (1:1) (9CI) (CA INDEX NAME)

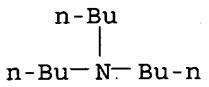
CM 1

CRN 1984-15-2
CMF C H6 O6 P2



CM 2

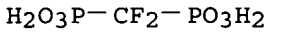
CRN 102-82-9
CMF C12 H27 N



RN 209454-90-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:1) (9CI) (CA INDEX NAME)

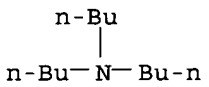
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2



CM 2

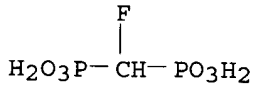
CRN 102-82-9
CMF C12 H27 N



RN 209454-91-1 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:1) (9CI) (CA INDEX NAME)

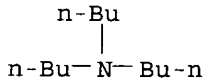
CM 1

CRN 10595-93-4
CMF C H5 F O6 P2



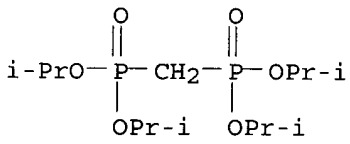
CM 2

CRN 102-82-9
CMF C12 H27 N

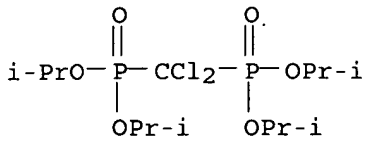


REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

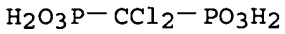
L17 ANSWER 8 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1998:332478 HCAPLUS
DOCUMENT NUMBER: 129:41194
TITLE: Synthesis of oxidronate
AUTHOR(S): Hu, Ming-Ying; Liang, Gao-Lin; Yang, Ming; Yu, Yan-Hua
CORPORATE SOURCE: Jiangsu Institute of Nuclear Medicine, State Key Laboratory of Nuclear Medicine, Wuxi, 214063, Peop. Rep. China
SOURCE: Zhongguo Yiyao Gongye Zazhi (1998), 29(1), 3-4
CODEN: ZYGZEA; ISSN: 1001-8255
PUBLISHER: Zhongguo Yiyao Gongye Zazhi Bianjibu
DOCUMENT TYPE: Journal
LANGUAGE: Chinese
AB Sodium oxidronate was prepared from triisopropyl phosphite by diphosphonation, chlorination, pyrolysis and reduction with 32% overall yield.
IT **1660-95-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and chlorination of)
RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



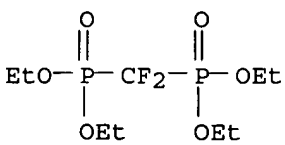
IT **10596-22-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and deesterification of)
RN 10596-22-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **10596-23-3P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and pyrolysis of)
RN 10596-23-3 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis- (9CI) (CA INDEX NAME)



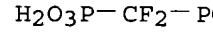
L17 ANSWER 9 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1997:721703 HCAPLUS
DOCUMENT NUMBER: 127:331684
TITLE: ATP analogs with non-transferable groups in the γ position as inhibitors of glycerol kinase
AUTHOR(S): Bystrom, Cory E.; Pettigrew, Donald W.; Remington, S. James; Branchaud, Bruce P.
CORPORATE SOURCE: Institute of Molecular Biology, Dep. of Chemistry and Dep. of Physics, University of Oregon, Eugene, OR, 97403, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1997), 7(20), 2613-2616
CODEN: BMCLE8; ISSN: 0960-894X
PUBLISHER: Elsevier
DOCUMENT TYPE: Journal
LANGUAGE: English
AB β,γ-Difluoromethyleneadenosine-5'-triphosphate (AMP-PCF2P) and γ-arsono-β,γ-methyleneadenosine-5'-diphosphate (AMP-PCAs) were synthesized and found to be competitive inhibitors of glycerol kinase. Com. available AMP-PCP and AMP-PNP also are competitive inhibitors. The structural similarities and differences of these ATP analogs and their effect on kinase inhibition are discussed.
IT **78715-58-9P 198011-41-5P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); **PREP (Preparation)**; **RACT (Reactant or reagent)**
(ATP analogs with non-transferable groups as inhibitors of glycerol kinase)
RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



RN 198011-41-5 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (1:4) (9CI) (CA INDEX NAME)

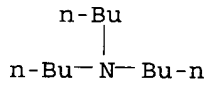
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2



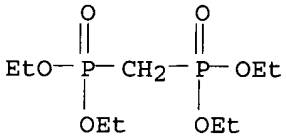
CM 2

CRN 102-82-9
CMF C12 H27 N

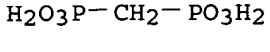


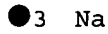
REFERENCE COUNT: 12 THERE ARE 12 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 10 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:551070 HCAPLUS
DOCUMENT NUMBER: 117:151070
TITLE: Synthesis and heteronuclear NMR analysis of deuterium- and tritium-labeled methylenebisphosphonic acid
AUTHOR(S): Blackburn, G. Michael; Rozenberg, S. G.; Yakovleva, G. M.
CORPORATE SOURCE: Krebs Inst., Univ. Sheffield, Sheffield, S3 7HF, UK
SOURCE: Tetrahedron Letters (1992), 33(27), 3927-30
CODEN: TELEAY; ISSN: 0040-4039
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Deuterium was substituted into the methylene group of methylenebisphosphonic acid (MDP) by metalation of (EtO)2P(O)CH2P(O)(OEt)2 with NaH in toluene followed by quenching with D2O. Anal. of the phosphorus NMR spectrum of the product shows a linear high-frequency shift on sequential mono- and dideuteration. The corresponding tritium labeling of MDP achieved a specific activity of 30 mCi/mmol.
IT **1660-94-2**, Tetraethyl methylenebisphosphonate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(metalation with sodium hydride and sequential deuteration of)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)

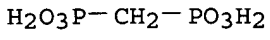


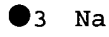
IT **39478-93-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and deuteration of)
RN 39478-93-8 HCAPLUS
CN Phosphonic acid, methylenebis-, trisodium salt (9CI) (CA INDEX NAME)



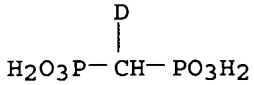


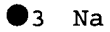
IT **143521-51-1P 143521-77-1P 143521-78-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 143521-51-1 HCAPLUS
CN Phosphonic acid, 1-methylenebis-, labeled with tritium, trisodium salt (9CI) (CA INDEX NAME)



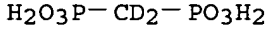


RN 143521-77-1 HCAPLUS
CN Phosphonic acid, methylene-d-bis-, trisodium salt (9CI) (CA INDEX NAME)



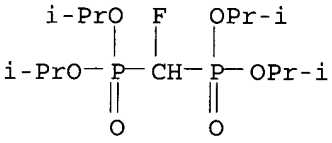


RN 143521-78-2 HCAPLUS
CN Phosphonic acid-d, methylene-d2-bis-, trisodium salt (9CI) (CA INDEX NAME)



L17 ANSWER 11 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1992:120437 HCAPLUS
DOCUMENT NUMBER: 116:120437

TITLE: Synthesis of a difluoromethylenephosphonate analog of AZT 5'-triphosphate and its inhibition of HIV-1 reverse transcriptase
AUTHOR(S): Hebel, D.; Kirk, K. L.; Kinjo, J.; Kovacs, T.; Lesiak, K.; Balzarini, J.; De Clercq, E.; Torrence, P. F.
CORPORATE SOURCE: Lab. Bioorg. Chem., Natl. Inst. Diabetes Dig. Kidney Dis., Bethesda, MD, 20892, USA
SOURCE: Bioorganic & Medicinal Chemistry Letters (1991), 1(7), 357-60
CODEN: BMCLE8; ISSN: 0960-894X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB Difluoromethylenebisphosphonic acid was prepared by acetyl hypofluorite-mediated fluorination of tetraisopropyl methylenebisphosphonate and ester hydrolysis. Coupling to 3'-azido-3'-deoxythymidine 5'-monophosphate gave the title compound The difluoromethylenephosphate was 30-fold less effective than AZT-triphosphate as a competitive inhibitor of HIV-1 reverse transcriptase but 10-fold more effective than the methylenephosphonate analog.
IT **78715-57-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(anion formation and fluorination of)
RN 78715-57-8 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **10596-32-4P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, with azidothymidinephosphoromorpholidate)
RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)

L17 ANSWER 12 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:449979 HCAPLUS
DOCUMENT NUMBER: 115:49979
TITLE: Process for the preparation of methylenebisphosphonic acids from the tetraesters using diluted hydrochloric acid
INVENTOR(S): Lampi, Klaus; Nieminen, Kauko; Ruohonen, Jarkko
PATENT ASSIGNEE(S): Huhtamaki Oy, Finland
SOURCE: PCT Int. Appl., 11 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9103480	A1	19910321	WO 1990-FI197	19900815
W: AU, CA, JP, NO, SU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
FI 83657	B	19910430	FI 1989-4245	19890908
FI 8904245	A	19910309		
FI 83657	C	19910812		
AU 9061582	A1	19910408	AU 1990-61582	19900815
AU 640884	B2	19930902		
EP 490907	A1	19920624	EP 1990-912071	19900815
EP 490907	B1	19941221		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, NL, SE				
JP 05504943	T2	19930729	JP 1990-511215	19900815
JP 2835651	B2	19981214		
ES 2067040	T3	19950316	ES 1990-912071	19900815
CA 2066430	C	19990202	CA 1990-2066430	19900815
ZA 9006720	A	19910626	ZA 1990-6720	19900823
NO 9200892	A	19920306	NO 1992-892	19920306
NO 180378	B	19961230		
NO 180378	C	19970409		
RU 2041230	C1	19950809	RU 1992-5011701	19920306
US 5237094	A	19930817	US 1992-838422	19920430

PRIORITY APPLN. INFO.: FI 1989-4245 A 19890908
WO 1990-FI197 A 19900815

OTHER SOURCE(S): MARPAT 115:49979

AB R1R2C(PO3H2)2 (R1, R2 = H, halo) were prepared by hydrolysis of R1R2C(PO3R32)2 (R3 = C1-4 alkyl) in 1.0-5% aqueous HCl, with optional conversion of the free acid to a salt via base treatment. Thus, a mixture of Cl2C[PO3(CHMe2)2]2 in .apprx.2-6 weight % HCl was refluxed followed by treatment with activated C and NaOH to pH 3.2 to give Cl2C(PO3H2)2 disodium tetrahydrate.

IT **7647-01-0**, Hydrochloric acid, reactions
RL: RCT (Reactant); RACT (Reactant or reagent)
(hydrolysis by diluted, of methylenebisphosphonate tetraesters)

RN 7647-01-0 HCAPLUS

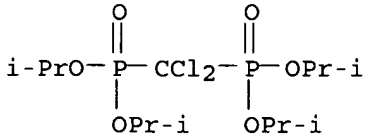
CN Hydrochloric acid (6CI, 7CI, 8CI, 9CI) (CA INDEX NAME)

HCl

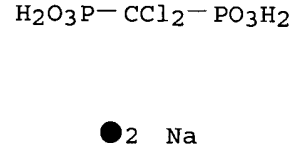
IT **10596-22-2**, Tetraisopropyl dichloromethylenebisphosphonate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(hydrolysis of, with diluted hydrochloric acid)

RN 10596-22-2 HCAPLUS

CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **22560-50-5P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, by hydrolysis of tetraisopropyl ester with diluted hydrochloric acid)
RN 22560-50-5 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, disodium salt (9CI) (CA INDEX NAME)



L17 ANSWER 13 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1991:229151 HCAPLUS
DOCUMENT NUMBER: 114:229151
TITLE: Preparation of novel halomethylenebisphosphonate partial esters as drugs
INVENTOR(S): Pohjala, Esko; Nupponen, Heikki; Vepsalainen, Jouko
PATENT ASSIGNEE(S): Huhtamaki Oy, Finland
SOURCE: PCT Int. Appl., 64 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 9015806	A1	19901227	WO 1990-FI163	19900619
W: AU, BG, BR, CA, FI, HU, JP, KP, KR, NO, RO, SU, US				
RW: AT, BE, CH, DE, DK, ES, FR, GB, IT, LU, NL, SE				
FI 8903039	A	19901222	FI 1989-3039	19890621
FI 83421	B	19910328		
FI 83421	C	19910710		
CA 2062735	AA	19901222	CA 1990-2062735	19900619
CA 2062735	C	20000815		
AU 9058272	A1	19910108	AU 1990-58272	19900619
AU 633459	B2	19930128		
EP 479813	A1	19920415	EP 1990-909051	19900619
EP 479813	B1	19950920		
R: AT, BE, CH, DE, DK, ES, FR, GB, IT, LI, LU, NL, SE				
JP 05500208	T2	19930121	JP 1990-508624	19900619
JP 2929236	B2	19990803		
HU 62008	A2	19930329	HU 1990-4623	19900619
HU 208701	B	19931228		
AT 128139	E	19951015	AT 1990-909051	19900619
ES 2078970	T3	19960101	ES 1990-909051	19900619
RU 2074860	C1	19970310	RU 1990-5010886	19900619
ZA 9004828	A	19910327	ZA 1990-4828	19900621
NO 9105021	A	19911219	NO 1991-5021	19911219
NO 178030	B	19951002		
NO 178030	C	19960110		
US 5376649	A	19941227	US 1992-777555	19920203
PRIORITY APPLN. INFO.:			FI 1989-3039 A	19890621

WO 1990-FI163 A 19900619

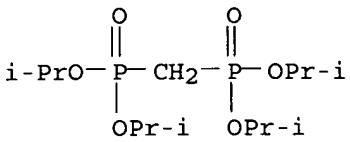
OTHER SOURCE(S): MARPAT 114:229151

AB (R1O)R2OP(O)CR5R6P(O)(OR3)OR4 [I; R1-R4 = H, silyl, (cyclo)alkyl, (cyclo)alkenyl, alkynyl, aryl(alkyl); ≥1 of R1-R4 = H, ≥1 of R1-R4 ≠ H; R5 = Cl, Br, iodo; R6 = R5, H, F], were prepared for treatment of disorders of bivalent metal metabolism (no data). Thus, I [R1-R4 = Me(CH2)5, R5 = R6 = Cl] (preparation given) was refluxed 1 h in pyridine to give the trihexyl derivative as a pyridinium salt, which was converted to I [R1 = R2 = R3 = Me(CH2)5, R4 = Na, R5 = R6 = Cl].

IT **1660-95-3**, Tetraisopropyl methylenebisphosphonate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(chlorination of, in preparation of drug)

RN 1660-95-3 HCAPLUS

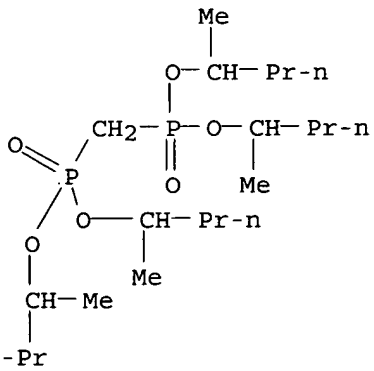
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **1498-95-9P 1643-14-7P**, Tetrapentyl methylenebisphosphonate **1660-94-2P**, Tetraethyl methylenebisphosphonate **1660-95-3P**, Tetraisopropyl methylenebisphosphonate **3011-78-7P**, Tetrahexyl methylenebisphosphonate **6997-56-4P**, Tetrabutyl methylenebisphosphonate **16001-93-7P**, Tetramethyl methylenebisphosphonate **25091-05-8P 109491-54-5P**, Tetraheptyl methylenebisphosphonate **133918-43-1P 133918-45-3P 133918-46-4P 133918-47-5P 133918-65-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and chlorination of)

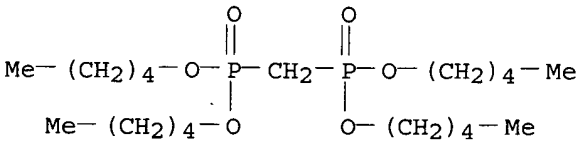
RN 1498-95-9 HCAPLUS

CN Phosphonic acid, methylenebis-, tetrakis(1-methylbutyl) ester (9CI) (CA INDEX NAME)

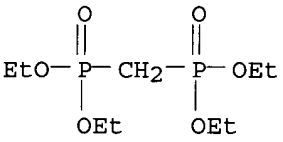


RN 1643-14-7 HCAPLUS

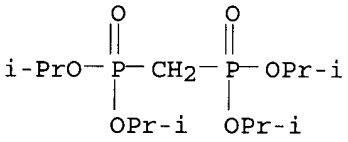
CN Phosphonic acid, methylenebis-, tetrapentyl ester (9CI) (CA INDEX NAME)



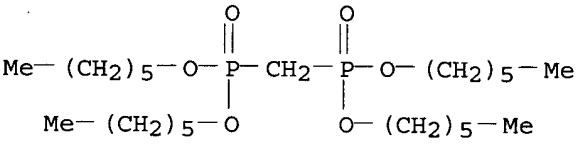
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



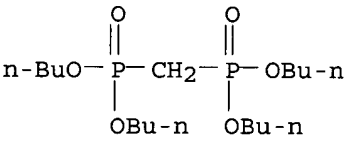
RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



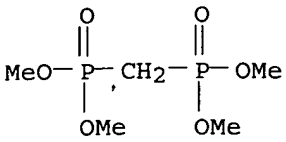
RN 3011-78-7 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrahexyl ester (9CI) (CA INDEX NAME)



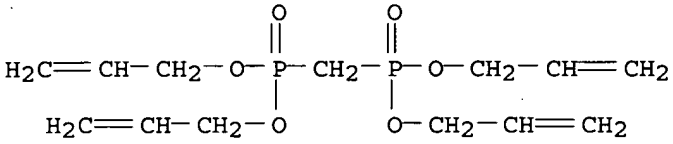
RN 6997-56-4 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrabutyl ester (9CI) (CA INDEX NAME)



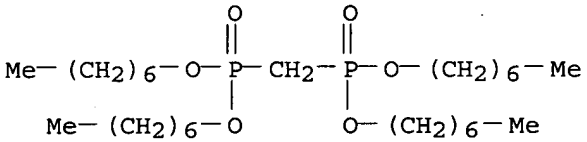
RN 16001-93-7 HCAPLUS
CN Phosphonic acid, methylenebis-, tetramethyl ester (9CI) (CA INDEX NAME)



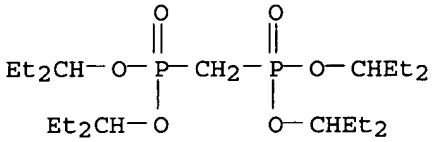
RN 25091-05-8 HCAPLUS
CN Phosphonic acid, methylenebis-, tetra-2-propenyl ester (9CI) (CA INDEX NAME)



RN 109491-54-5 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraheptyl ester (9CI) (CA INDEX NAME)

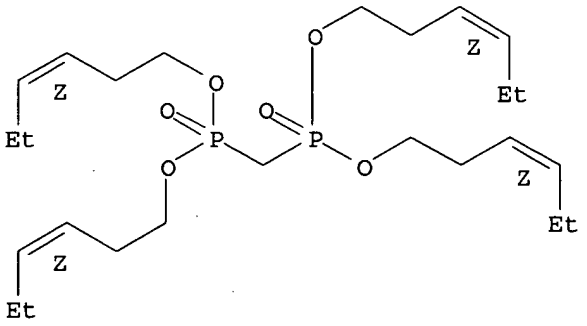


RN 133918-43-1 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-ethylpropyl) ester (9CI) (CA INDEX NAME)

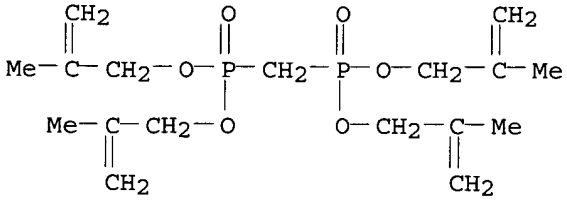


RN 133918-45-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetra-3-hexenyl ester, (all-Z)- (9CI) (CA INDEX NAME)

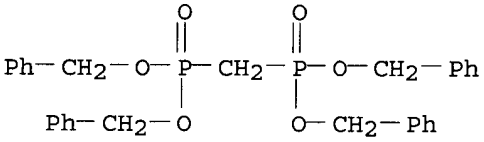
Double bond geometry as shown.



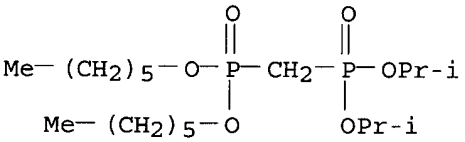
RN 133918-46-4 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(2-methyl-2-propenyl) ester (9CI) (CA INDEX NAME)



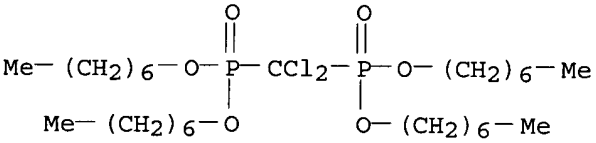
RN 133918-47-5 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(phenylmethyl) ester (9CI) (CA INDEX NAME)



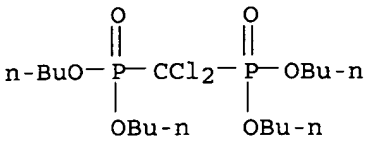
RN 133918-65-7 HCAPLUS
CN Phosphonic acid, [[bis(hexyloxy)phosphinyl]methyl]-, bis(1-methylethyl) ester (9CI) (CA INDEX NAME)



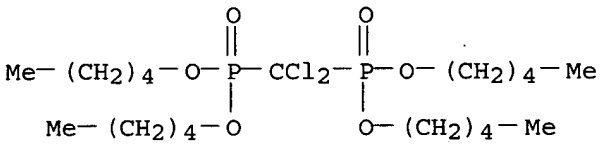
IT **27291-41-4P**, Tetraheptyl dichloromethylenebisphosphonate
133918-51-1P, Tetrabutyl dichloromethylenebisphosphonate
133918-52-2P, Tetrapentyl dichloromethylenebisphosphonate
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and partial hydrolysis of, in preparation of drug)
RN 27291-41-4 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetraheptyl ester (9CI) (CA INDEX NAME)



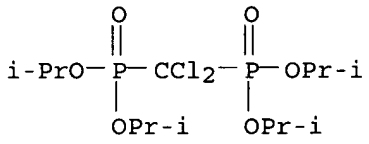
RN 133918-51-1 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrabutyl ester (9CI) (CA INDEX NAME)



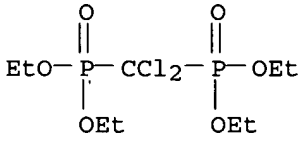
RN 133918-52-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrapentyl ester (9CI) (CA INDEX NAME)



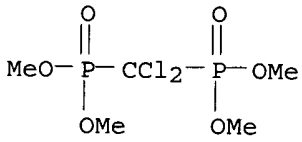
IT **10596-22-2P**, Tetraisopropyl dichloromethylenebisphosphonate
19928-97-3P, Tetraethyl dichloromethylenebisphosphonate
19929-29-4P, Tetramethyl dichloromethylenebisphosphonate
19929-31-8P 20107-67-9P 133918-42-0P
133918-48-6P 133918-50-0P 133918-53-3P
133918-54-4P 133918-56-6P 133918-57-7P
133918-58-8P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and partial saponification of, in preparation of drug)
RN 10596-22-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



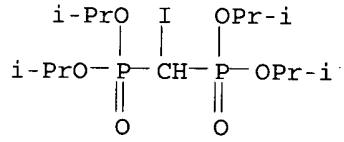
RN 19928-97-3 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



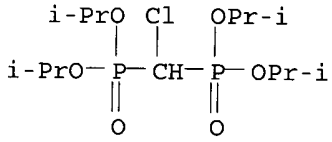
RN 19929-29-4 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetramethyl ester (9CI) (CA INDEX NAME)



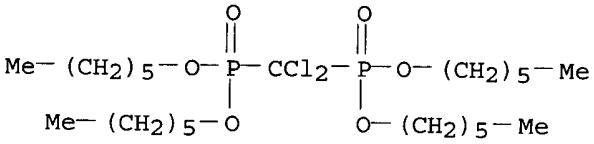
RN 19929-31-8 HCAPLUS
CN Phosphonic acid, (iodomethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



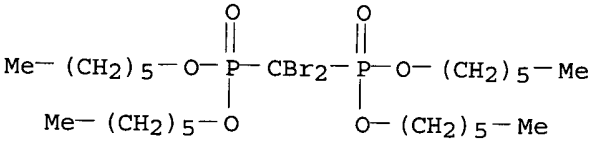
RN 20107-67-9 HCAPLUS
CN Phosphonic acid, (chloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



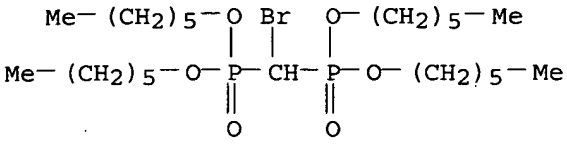
RN 133918-42-0 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrahexyl ester (9CI) (CA INDEX NAME)



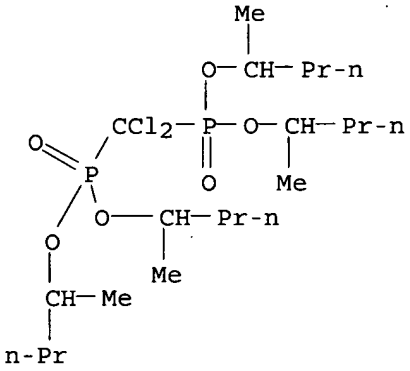
RN 133918-48-6 HCAPLUS
CN Phosphonic acid, (dibromomethylene)bis-, tetrahexyl ester (9CI) (CA INDEX NAME)



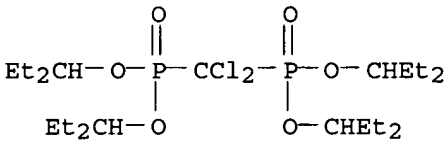
RN 133918-50-0 HCAPLUS
CN Phosphonic acid, (bromomethylene)bis-, tetrahexyl ester (9CI) (CA INDEX NAME)



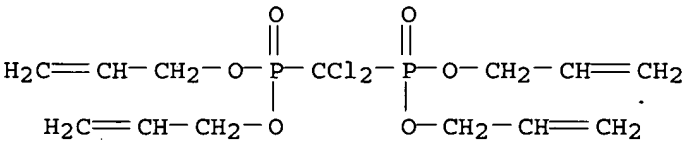
RN 133918-53-3 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylbutyl) ester (9CI) (CA INDEX NAME)



RN 133918-54-4 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-ethylpropyl) ester (9CI) (CA INDEX NAME)

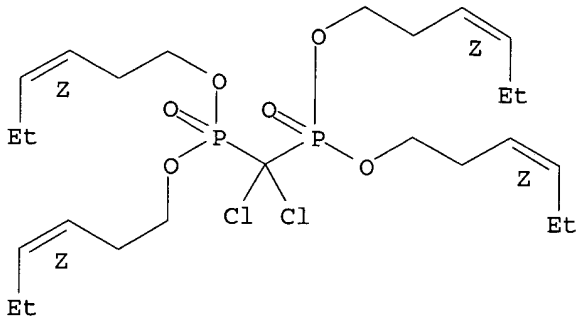


RN 133918-56-6 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetra-2-propenyl ester (9CI) (CA INDEX NAME)

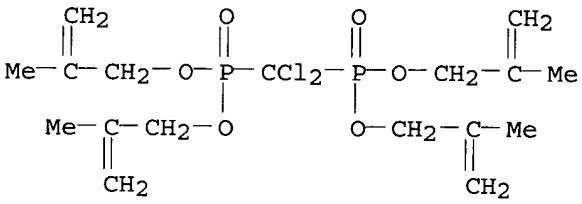


RN 133918-57-7 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetra-3-hexenyl ester, (all-Z)- (9CI) (CA INDEX NAME)

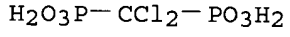
Double bond geometry as shown.

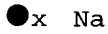


RN 133918-58-8 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(2-methyl-2-propenyl) ester (9CI) (CA INDEX NAME)

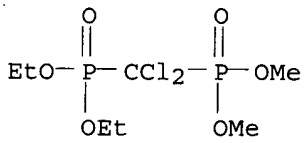


IT **29329-69-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, as drug intermediate)
RN 29329-69-9 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, sodium salt (9CI) (CA INDEX NAME)





IT **133918-66-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, in preparation of drug)
RN 133918-66-8 HCAPLUS
CN Phosphonic acid, [dichloro(diethoxyphosphinyl)methyl]-, dimethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 14 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1990:515623 HCAPLUS
DOCUMENT NUMBER: 113:115623
TITLE: Farnesyloxyphosphonylmethylphosphonates and analogs as squalene synthetase inhibitors
INVENTOR(S): Sofia, Michael J.; Biller, Scott A.
PATENT ASSIGNEE(S): E. R. Squibb and Sons, Inc., USA
SOURCE: Eur. Pat. Appl., 27 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 3
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 356866	A2	19900307	EP 1989-115400	19890821
EP 356866	A3	19910327		
R: DE, FR, GB, IT				
JP 02101088	A2	19900412	JP 1989-222777	19890829
PRIORITY APPLN. INFO.:			US 1988-237940 A	19880829
OTHER SOURCE(S):	MARPAT 113:115623			

AB Me2C:CHCH2CH2CMe:CHQ(CH2)nXP(O)(OR1)CR2R3P(O)(OR4)OR (I; Q = -CH2CH2CMe:CH, bond; n = 1-4; X = O, NH, NR5; R, R1, R4 = H, alkyl, alkenyl, metal ion; R2, R3 = H, halo; R5 = alkyl; when X = O, n = 2-4), useful as squalene synthetase inhibitors (no data), were prepared Thus, (MeO)2P(O)CH2P(O)(OMe)OH (preparation given) in CH2Cl2 containing (Me2CH)2NEt was treated with (PhO)2P(O)Cl; the mixture was stirred 2 h and farnesylamine (preparation from trans,trans-farnesol given) and (Me2CH)2NEt in CH2Cl2 was added at 0° to give 48% Me2C:CHCH2CH2CMe:CHCH2CH2CMe:CHCH2NHP(O)(OMe)CH2P(O)(OMe)2.

IT **93978-76-8P**
RL: RCT (Reactant); SPN (Synthetic preparation); **PREP (Preparation)**; RACT (Reactant or reagent)
(preparation and reaction of, in preparation of farnesyloxyphosphenylmethylphosphonic acid)

RN 93978-76-8 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, methylenebis[phosphonate] (3:1) (9CI) (CA INDEX NAME)

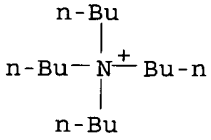
CM 1

CRN 93978-75-7
CMF C H3 O6 P2

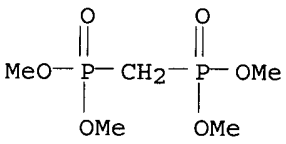
$^{-}HO_3P-CH_2-PO_3^{2-}$

CM 2

CRN 10549-76-5
CMF C16 H36 N



IT **16001-93-7**, Tetramethylmethylenediphosphonate
RL: **RCT (Reactant); RACT (Reactant or reagent)**
(reaction of, in preparation of squalene synthetase inhibitor)
RN 16001-93-7 HCAPLUS
CN Phosphonic acid, methylenebis-, tetramethyl ester (9CI) (CA INDEX NAME)

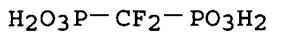


L17 ANSWER 15 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1990:473593 HCAPLUS
DOCUMENT NUMBER: 113:73593
TITLE: (Difluoromethylene)phosphates of guanine nucleosides as probes of DNA polymerases and G proteins
AUTHOR(S): Arabshahi, Lili; Khan, Naseema N.; Butler, Michelle; Noonan, Timothy; Brown, Neal C.; Wright, George E.
CORPORATE SOURCE: Med. Sch., Univ. Massachusetts, Worcester, MA, 01655, USA
SOURCE: Biochemistry (1990), 29(29), 6820-6
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English
AB 5'-Polyphosphates of N2-(p-n-butylphenyl)-2'-deoxyguanosine and -guanosine which contain a difluoromethylene group in place of a phosphoanhydide O atom were synthesized. 5'-[β,γ-(Difluoromethylene)triphosphate s), including that of 2'-deoxyguanosine, were prepared by reaction of the corresponding 5'-phosphates, activated by 1,1'-carbonyldiimidazole, with difluoromethanediphosphonate. The 5'-[(difluoromethylene)diphosphate] of N2-(p-n-butylphenyl)guanosine was prepared by treatment of a protected 5'-tosyl nucleoside with difluoromethanediphosphonate, followed by deprotection. Condensation of this nucleotide, activated with 1,1'-carbonyldiimidazole, with orthophosphate gave N2-(p-n-butylphenyl)guanosine 5'-[(α,β-difluoromethylene)triphosphate]. The products were characterized by 31P and 19F NMR spectroscopy. The phosphonates were tested for their ability to displace [3H)GDP from the GTP-binding proteins and cellular (EC) and oncogenic (Leu-61) Ha-ras p21, and for their ability to inhibit DNA polymerase-α from CHO cells. The proteins p21 bound weakly to a triphosphonate when the CF2 group was in the β,γ-position, but not when it was in the α,β-position, and they did not bind to corresponding (difluoromethylene)diphosphate. In contrast, the CF2 group had no effect on inhibition of DNA polymerase-α by N2-(p-n-butylphenyl-2'-deoxyguanosine 5'-[(β,γ-difluoromethylene)triphosphate]. 2'-Deoxyguanosine 5'-[(β,γ-difluoromethylene)triphosphate] was found to be a bona fide substrate for several DNA polymerases and had a lower apparent Km than dGTP with Bacillus subtilis DNA polymerase III.

IT **128360-68-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and condensation with guanine nucleosides)
RN 128360-68-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with N,N-dibutyl-1-butanamine (9CI) (CA INDEX NAME)

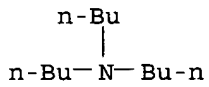
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2

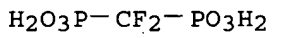


CM 2

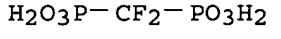
CRN 102-82-9
CMF C12 H27 N

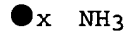


IT **10596-32-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and conversion to ammonium salt)
RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)



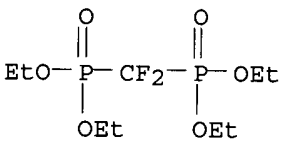
IT **128360-69-0P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and conversion to triethylammonium salt)
RN 128360-69-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, ammonium salt (9CI) (CA INDEX NAME)





IT **78715-58-9**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(reaction of, with iodotrimethylsilane)
RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA

INDEX NAME)



L17 ANSWER 16 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:587624 HCAPLUS
DOCUMENT NUMBER: 111:187624
TITLE: Bisphosphonates as bone reabsorption inhibitors
INVENTOR(S): Rosini, Sergio; Staibano, Giorgio
PATENT ASSIGNEE(S): Istituto Gentili S.p.A., Italy
SOURCE: U.S., 9 pp. Cont.-in-part of U.S. Ser. No. 480,264.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 2
PATENT INFORMATION:

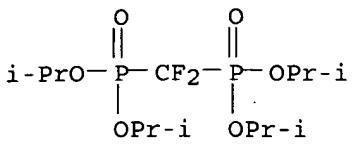
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4621077	A	19861104	US 1984-618578	19840608
CH 661437	A	19870731	CH 1983-1654	19830325
GB 2118042	A1	19831026	GB 1983-8791	19830330
GB 2118042	B2	19860115		
FR 2525223	A1	19831021	FR 1983-5858	19830411
FR 2525223	B1	19860425		
JP 58189193	A2	19831104	JP 1983-65160	19830413
JP 02013645	B4	19900404		
SE 8302130	A	19831016	SE 1983-2130	19830415
SE 463239	B	19901029		
SE 463239	C	19910221		
NL 8301324	A	19831101	NL 1983-1324	19830415
NL 192562	B	19970602		
NL 192562	C	19971003		

PRIORITY APPLN. INFO.: IT 1982-20781 A 19820415
US 1983-480264 A2 19830330

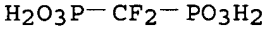
AB The bisphosphonic acids RR1C(PO3H2)2 (R = F, alkyl, aminoalkyl, fluoroalkyl; R1 = F, OH) and their salts, are prepared as drugs for the treatment of urolithiasis and as bone reabsorption inhibitors. A heated mixture of 4-aminobutyric acid, P(OH)3 and ClPh was treated with PCl3 to give 4-amino-1-hydroxybutane-1,1-bisphosphonic acid (I). Administration of 8 mg I/day to a patient with neoplastic hypercalcemia for 2 days decreased the blood Ca level from 14 to 9 mg%. In vitro and in vivo expts. indicated that I is 100-300-times more active as a bone reabsorption inhibitor than the standard Cl2C(PO3H2)2.

IT **78715-59-0P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and hydrolysis of)

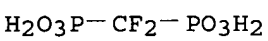
RN 78715-59-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **10596-32-4P 89732-98-9P 89732-99-0P**
123343-72-6P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of, for urolithiasis treatment and as bone readsorption inhibitor)
RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)



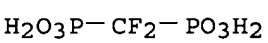
RN 89732-98-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, trisodium salt (9CI) (CA INDEX NAME)



RN 89732-99-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with benzenamine (1:4) (9CI) (CA INDEX NAME)

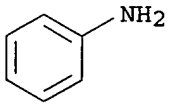
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2



CM 2

CRN 62-53-3
CMF C6 H7 N



RN 123343-72-6 HCAPLUS

CN L-Lysine, (difluoromethylene)bis[phosphonate] (2:1) (9CI) (CA INDEX NAME)

CM 1

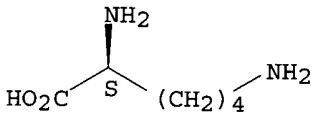
CRN 10596-32-4
CMF C H4 F2 O6 P2

$H_2O_3P-CF_2-PO_3H_2$

CM 2

CRN 56-87-1
CMF C6 H14 N2 O2

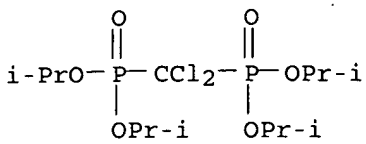
Absolute stereochemistry.



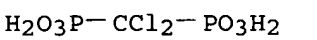
L17 ANSWER 17 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:569924 HCAPLUS
DOCUMENT NUMBER: 111:169924
TITLE: Carbonyldiphosphonate, a selective inhibitor of mammalian DNA polymerase δ
AUTHOR(S): Talanian, Robert V.; Brown, Neal C.; McKenna, Charles E.; Ye, Ting Gao; Levy, Jeffrey N.; Wright, George E.
CORPORATE SOURCE: Med. Sch., Univ. Massachusetts, Worcester, MA, 01655, USA
SOURCE: Biochemistry (1989), 28(21), 8270-4
CODEN: BICHAW; ISSN: 0006-2960
DOCUMENT TYPE: Journal
LANGUAGE: English

AB Twenty-three pyrophosphate analogs were screened as inhibitors of proliferating cell nuclear antigen-independent DNA polymerase δ (pol δ) derived from calf thymus. Carbonyldiphosphonate (COMDP), also known as α-oxomethylenediphosphonate, inhibited pol δ with a potency (Ki = 1.8 μM) 20-fold greater than that displayed for DNA polymerase α (pol α) derived from the same tissue. Characterization of the mechanism of inhibition of pol δ indicated that COMDP competed with the dNTP specified by the template and was not competitive with the template·primer. In the case of pol α, COMDP did not compete with either the dNTP or the polynucleotide substrate. COMDP inhibited the 3' → 5' exonuclease activity of pol δ weakly, displaying an IC50 >1 mM.

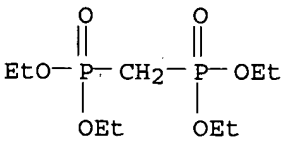
IT **10596-22-2**, Tetraisopropyl(dichloromethylene)diphosphonate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(deprotection of)
RN 10596-22-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **10596-23-3P**, (Dichloromethylene)diphosphonic acid
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and conversion to carbonyldiphosphonate)
RN 10596-23-3 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis- (9CI) (CA INDEX NAME)

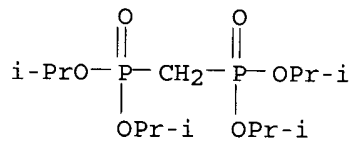


L17 ANSWER 18 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1989:407503 HCAPLUS
DOCUMENT NUMBER: 111:7503
TITLE: Synthesis of α-halogenated methanediphosphonates
AUTHOR(S): McKenna, Charles E.; Khawli, Leslie A.; Ahmad, Wan Yaacob; Pham Phuong; Bongartz, Jean Pierre
CORPORATE SOURCE: Dep. Chem., Univ. South. California, Los Angeles, CA, 90089-0744, USA
SOURCE: Phosphorus and Sulfur and the Related Elements (1988), 37(1-2), 1-12
CODEN: PREEDF; ISSN: 0308-664X
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 111:7503
AB α-Halo-substitution of methanediphosphonate (MDP) anions provides MDP derivs. XX1MDP (X = H, F, Cl, Br; X1 = F, Cl, Br) with modified acid-base, steric and other properties. These compds. are conveniently made from the corresponding α-halogenated XX1MDP esters (RO)2P(O)CXX1P(O)(OR)2. Detailed procedures are given for synthesis of R4XX1MDP (R = CHMe2, Et, Me. NMR data (1H, 31P, 13C, 19F) are presented for the products obtained. The XX1MDP acids (X,X1 = H, Cl; Cl, Cl; H, Br; Br, Br; F, Cl; F, Br; Cl, Br) were prepared by HCl hydrolysis of a corresponding ester and characterized as tris(dicyclohexylammonium) salts by elemental analyses and 31P NMR.
IT **1660-94-2 1660-95-3 16001-93-7 78715-56-7 78715-57-8**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(chlorination of, with sodium hypochlorite)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)

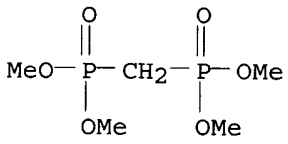


RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA

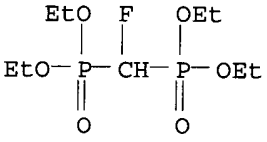
INDEX NAME)



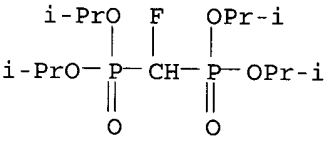
RN 16001-93-7 HCAPLUS
CN Phosphonic acid, methylenebis-, tetramethyl ester (9CI) (CA INDEX NAME)



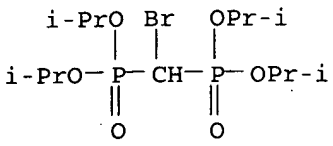
RN 78715-56-7 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



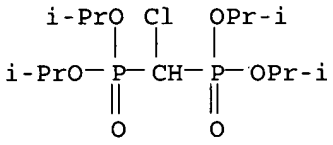
RN 78715-57-8 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



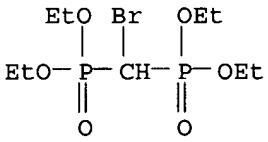
IT **10596-20-0P 20107-67-9P 28845-79-6P**
50870-71-8P 119351-13-2P 121151-56-2P
121151-57-3P
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and hydrolysis of)
RN 10596-20-0 HCAPLUS
CN Phosphonic acid, (bromomethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



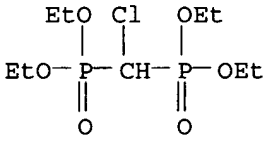
RN 20107-67-9 HCAPLUS
CN Phosphonic acid, (chloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



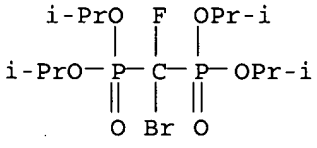
RN 28845-79-6 HCAPLUS
CN Phosphonic acid, (bromomethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



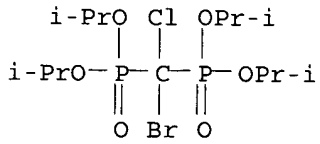
RN 50870-71-8 HCAPLUS
CN Phosphonic acid, (chloromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



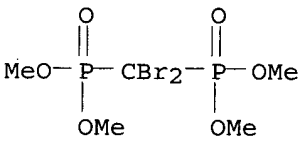
RN 119351-13-2 HCAPLUS
CN Phosphonic acid, (bromofluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



RN 121151-56-2 HCAPLUS
CN Phosphonic acid, (bromochloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



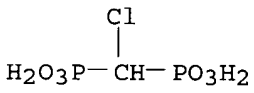
RN 121151-57-3 HCAPLUS
CN Phosphonic acid, (dibromomethylene)bis-, tetramethyl ester (9CI) (CA INDEX NAME)



IT **121151-58-4P 121151-59-5P 121151-60-8P**
121151-61-9P 121151-62-0P 121151-63-1P
121151-64-2P
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 121151-58-4 HCAPLUS
CN Phosphonic acid, (chloromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:2) (9CI) (CA INDEX NAME)

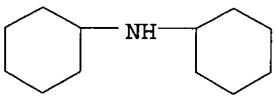
CM 1

CRN 87591-00-2
CMF C H5 Cl O6 P2



CM 2

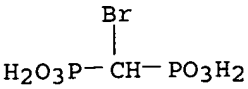
CRN 101-83-7
CMF C12 H23 N



RN 121151-59-5 HCAPLUS
CN Phosphonic acid, (bromomethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

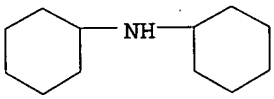
CM 1

CRN 10596-21-1
CMF C H5 Br O6 P2



CM 2

CRN 101-83-7
CMF C12 H23 N



RN 121151-60-8 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

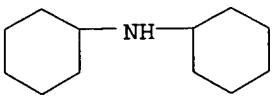
CM 1

CRN 10596-23-3
CMF C H4 Cl2 O6 P2

$H_2O_3P-CCl_2-PO_3H_2$

CM 2

CRN 101-83-7
CMF C12 H23 N



RN 121151-61-9 HCAPLUS
CN Phosphonic acid, (dibromomethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

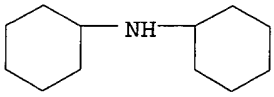
CM 1

CRN 10596-26-6
CMF C H4 Br2 O6 P2

$H_2O_3P-CBr_2-PO_3H_2$

CM 2

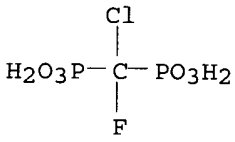
CRN 101-83-7
CMF C12 H23 N



RN 121151-62-0 HCAPLUS
CN Phosphonic acid, (chlorofluoromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

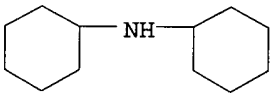
CM 1

CRN 111863-43-5
CMF C H4 Cl F O6 P2



CM 2

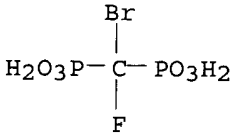
CRN 101-83-7
CMF C12 H23 N



RN 121151-63-1 HCAPLUS
CN Phosphonic acid, (bromofluoromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

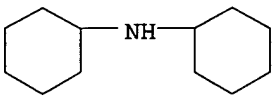
CM 1

CRN 111863-45-7
CMF C H4 Br F O6 P2



CM 2

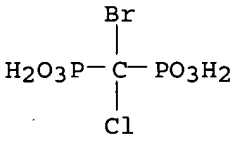
CRN 101-83-7
CMF C12 H23 N



RN 121151-64-2 HCAPLUS
CN Phosphonic acid, (bromochloromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

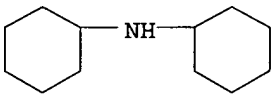
CM 1

CRN 111863-47-9
CMF C H4 Br Cl O6 P2

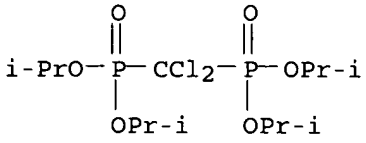


CM 2

CRN 101-83-7
CMF C12 H23 N



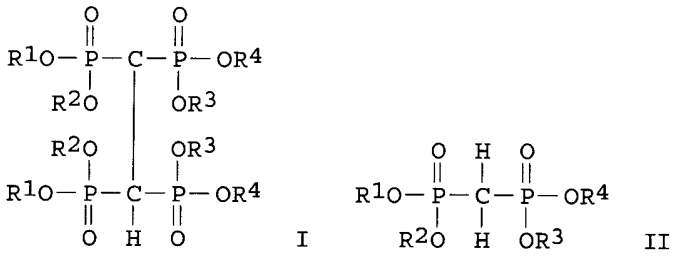
IT **10596-22-2P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation, hydrolysis, and reductive dechlorination of)
RN 10596-22-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



L17 ANSWER 19 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1988:13082 HCAPLUS
DOCUMENT NUMBER: 108:13082
TITLE: Novel tetraphosphonic acid compounds, intermediates and an electrochemical process for their production
INVENTOR(S): Noding, Stephen A.
PATENT ASSIGNEE(S): Dow Chemical Co., USA
SOURCE: U.S., 6 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4689123	A	19870825	US 1986-945729	19861223
PRIORITY APPLN. INFO.:			US 1986-945729	19861223

GI

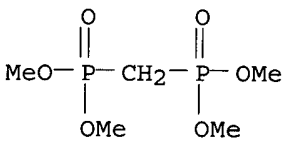


I II

AB Compds. I, in which R1, R2, R3, and R4 are each independently selected from H, Me3Si, and C1-20 alkyl groups are electrochem. prepared Ethylene tetraphosphonic acid is prepared by (a) electrolytically coupling a diphosphonate compound II, in which R1, R2, R3, and R4 are each independently selected from C1-20 alkyl groups, dissolved in a polar solvent (e.g. MeCN), in the presence of a quaternary NH4+ halide, to form an octaalkyl ethanetetraphosphonate ester; (b) converting the ester to its corresponding trimethylsilyl ester by reacting it with iodotrimethylsilane; and (c) hydrolyzing the resulting ester with H2O to form a composition containing ethylene tetraphosphonic acid.

IT **16001-93-7**, Tetramethyl methylene diphosphonate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(electrochem. coupling of, for preparation of tetraphosphonic acids)

RN 16001-93-7 HCAPLUS
CN Phosphonic acid, methylenebis-, tetramethyl ester (9CI) (CA INDEX NAME)



IT **1984-15-2P**, Methylene diphosphonic acid

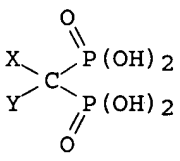
RL: FORM (Formation, nonpreparative); **PREP (Preparation)**
(formation of, in electrochem. coupling of diphosphonates)
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)

$H_2O_3P-CH_2-PO_3H_2$

L17 ANSWER 20 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:102549 HCAPLUS
DOCUMENT NUMBER: 106:102549
TITLE: Hydrolyzing substituted methylenediphosphonic acid esters
INVENTOR(S): Staibano, Giorgio
PATENT ASSIGNEE(S): Istituto Gentili S.p.A., Italy
SOURCE: Eur. Pat. Appl., 8 pp.
CODEN: EPXXDW
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

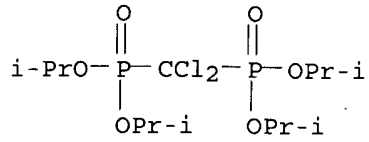
PATENT NO.	KIND	DATE	APPLICATION NO.		DATE
EP 200980	A1	19861112	EP 1986-105502		19860421
EP 200980	B1	19900131			
R: AT, BE, CH, DE, FR, GB, LI, LU, NL, SE					
AT 49975	E	19900215	AT 1986-105502		19860421
PRIORITY APPLN. INFO.:			IT 1985-20543	A	19850430
			EP 1986-105502	A	19860421

GI

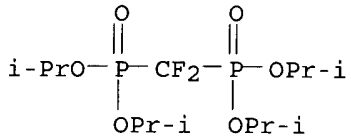


I

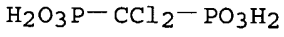
AB The title compds. I (X, Y = H, halo, alkyl) are prepared by hydrolysis of the corresponding tetraesters. Thus, 50 g Cl2C[P(O)(OCHMe2)2]2 was hydrolyzed at 80-100° in H2O to give 41.5 g I (X = Y = Cl), isolated as the di-Na salt.
IT **10596-22-2**, Tetraisopropyl dichloromethylenediphosphonate
78715-59-0, Tetraisopropyl difluoromethylenediphosphonate
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrolysis of)
RN 10596-22-2 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



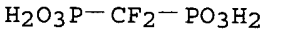
RN 78715-59-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



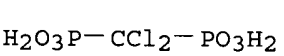
IT **10596-23-3P**, Dichloromethylenediphosphonic acid
10596-32-4P, Difluoromethylenediphosphonic acid
22560-50-5P, Disodium dichloromethylenediphosphonate
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 10596-23-3 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis- (9CI) (CA INDEX NAME)

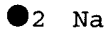


RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)



RN 22560-50-5 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis-, disodium salt (9CI) (CA INDEX NAME)





L17 ANSWER 21 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1987:5234 HCAPLUS
DOCUMENT NUMBER: 106:5234
TITLE: Phosphorylation of isoprenoid alcohols
AUTHOR(S): Davisson, V. Jo; Woodside, Andrew B.; Neal, Timothy R.; Stremler, Kay E.; Muehlbacher, Manfred; Poulter, C. Dale
CORPORATE SOURCE: Dep. Chem., Univ. Utah, Salt Lake City, UT, 84112, USA

SOURCE: Journal of Organic Chemistry (1986), 51(25), 4768-79
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 106:5234

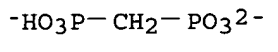
AB Procedures for the synthesis and purification of 20 isoprenoid diphosphates and methanediphosphonate analogs from the corresponding alcs., e.g., prenol, geraniol, farnesol, geranylgeraniol, are described. The alcs. are activated for phosphorylation by conversion of homoallylic systems to tosylates and allylic systems to halides. The activated intermediates are treated with tris(tetra-n-butylammonium) salts of pyrophosphoric, methanediphosphonic, or difluoromethanediphosphonic acid to obtain the corresponding esters in yields of 34-80%. Chromatog. on cellulose is a general method for purification of isoprenoid diphosphates, and procedures are described for compds. with C5 to C20 hydrocarbon moieties. The displacement by pyrophosphate occurs with inversion of configuration, and the procedure can be used to prepare isoprenoid diphosphates with chiral C-1 methylene groups in high optical purity from the corresponding alcs.

IT **93978-76-8P 104714-96-7P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and phosphorylation by, of isoprenoid alcs., via activated intermediates)

RN 93978-76-8 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, methylenebis[phosphonate] (3:1) (9CI) (CA INDEX NAME)

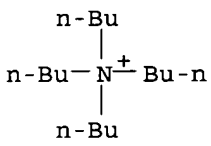
CM 1

CRN 93978-75-7
CMF C H3 O6 P2



CM 2

CRN 10549-76-5
CMF C16 H36 N



RN 104714-96-7 HCAPLUS
CN 1-Butanaminium, N,N,N-tributyl-, (difluoromethylene)bis[phosphonate] (3:1) (9CI) (CA INDEX NAME)

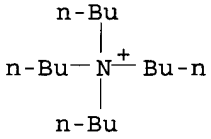
CM 1

CRN 104714-95-6
CMF C H F2 O6 P2

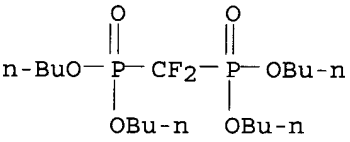
$^{-}HO_3P-CF_2-PO_3^{2-}$

CM 2

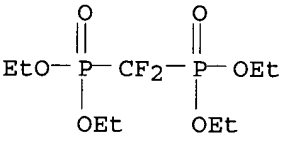
CRN 10549-76-5
CMF C16 H36 N



IT **74860-86-9P 78715-58-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction of, with bromotrimethylsilane)
RN 74860-86-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetrabutyl ester (9CI) (CA INDEX NAME)



RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



L17 ANSWER 22 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1985:95821 HCAPLUS
DOCUMENT NUMBER: 102:95821
TITLE: α-Fluorinated alkanediphosphonates
INVENTOR(S): McKenna, Charles E.
PATENT ASSIGNEE(S): University of Southern California, USA
SOURCE: U.S., 5 pp.
CODEN: USXXAM
DOCUMENT TYPE: Patent
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

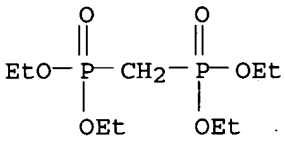
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 4478763	A	19841023	US 1982-435578	19821020

PRIORITY APPLN. INFO.: US 1982-435578 19821020
OTHER SOURCE(S): CASREACT 102:95821

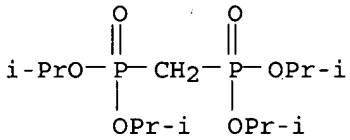
AB Several α-fluorinated methanediphosphonates were prepared by treating a methanediphosphonate ester (RO)2P(O)CH2P(O)(OR1)2 (R, R1 = aryl, alkyl) with KOCMe3, then with FClO3. Thus, treating (EtO)2P(O)CH2P(O)(OEt)2 in PhMe with KOCMe3, then with FClO3 gave 34% (EtO)2P(O)CHFP(O)(OEt)2, 21% (EtO)2P(O)CF2P(O)(OEt)2, and 7% (EtO)2P(O)CHF2. The product esters may be hydrolyzed.

IT **1660-94-2 1660-95-3 62285-41-0**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(fluorination of, with potassium tert-butoxide and perchloryl fluoride)

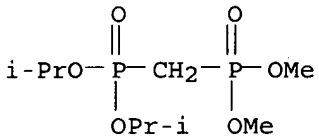
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)

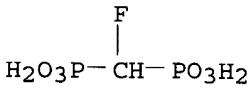


RN 62285-41-0 HCAPLUS
CN Phosphonic acid, [[bis(1-methylethoxy)phosphinyl]methyl]-, dimethyl ester (9CI) (CA INDEX NAME)



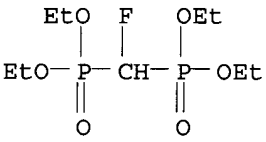
IT **10595-93-4P 10596-32-4P**
RL: PRP (Properties); SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and acidity of, theor. calcns. of)

RN 10595-93-4 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis- (9CI) (CA INDEX NAME)

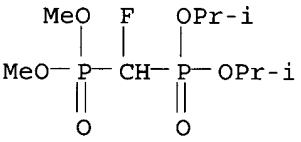


RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)

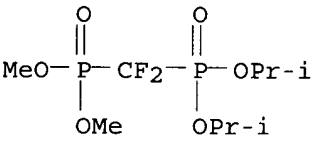
IT **78715-56-7P 95015-00-2P 95015-01-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction of, with bromotrimethylsilane)
RN 78715-56-7 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



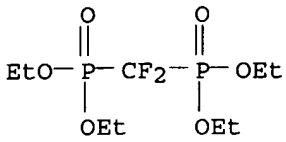
RN 95015-00-2 HCAPLUS
CN Phosphonic acid, [[bis(1-methylethoxy)phosphinyl]fluoromethyl]-, dimethyl ester (9CI) (CA INDEX NAME)



RN 95015-01-3 HCAPLUS
CN Phosphonic acid, [[bis(1-methylethoxy)phosphinyl]difluoromethyl]-, dimethyl ester (9CI) (CA INDEX NAME)



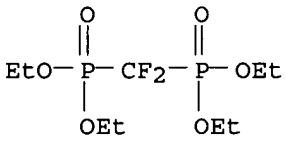
IT **78715-58-9P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and reaction with bromotrimethylsilane)
RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



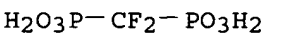
L17 ANSWER 23 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1983:54013 HCAPLUS
DOCUMENT NUMBER: 98:54013
TITLE: Preparation, stability and acidity of difluoromethylenebisphosphonic acid
AUTHOR(S): Burton, D. J.; Pietrzyk, D. J.; Ishihara, T.; Fonong, T.; Flynn, R. M.
CORPORATE SOURCE: Dep. Chem., Univ. Iowa, Iowa City, IA, 52242, USA
SOURCE: Journal of Fluorine Chemistry (1982), 20(5), 617-26
CODEN: JFLCAR; ISSN: 0022-1139
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 98:54013

AB Hydrolysis of (EtO)2P(O)CF2P(O)(OEt)2 via the trimethylsilyl ester quant. yields (HO)2P(O)CF2P(O)(OH)2 as a dihdyrate. In vacuo drying leads to either the monohydrate or the anhydrous acid. Titration of either the free acid or its disodium salt and computer fit of the data gives all four pKa's. The disodium salt and the free acid are thermally stable, and the disodium salt is extremely stable even to strong base.

IT **78715-58-9**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrolysis of, via trimethylsilyl ester)
RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



IT **10596-32-4P 84228-60-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation, acidity, and stability of)
RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)

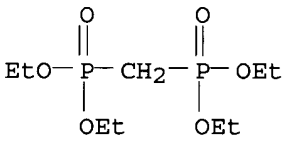


RN 84228-60-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, disodium salt (9CI) (CA INDEX NAME)

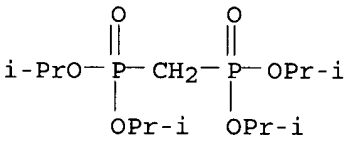
$H_2O_3P-CF_2-PO_3H_2$

●2 Na

L17 ANSWER 24 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1981:569297 HCAPLUS
DOCUMENT NUMBER: 95:169297
TITLE: Fluorination of methanediphosphonate esters by perchloryl fluoride. Synthesis of fluoromethanediphosphonic acid and difluoromethanediphosphonic acid
AUTHOR(S): McKenna, Charles E.; Shen, Pei-De
CORPORATE SOURCE: Dep. Chem., Univ. South. California, Los Angeles, CA, 90007, USA
SOURCE: Journal of Organic Chemistry (1981), 46(22), 4573-6
CODEN: JOCEAH; ISSN: 0022-3263
DOCUMENT TYPE: Journal
LANGUAGE: English
OTHER SOURCE(S): CASREACT 95:169297
AB Fluorination of [(RO)2P(O)]2CH2 (R = Et, Me2CH) with FClO3 gave [(RO)2P(O)]2CFR1 (R1 = H, F) which on transesterification with BrSiMe3 followed by hydrolysis gave [(HO)2P(O)]2CFR1.
IT **1660-94-2 1660-95-3**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(fluorination of)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)

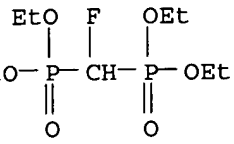


RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)

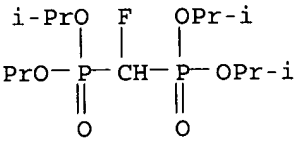


IT **78715-56-7P 78715-57-8P 78715-58-9P 78715-59-0P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and transesterification of)
RN 78715-56-7 HCAPLUS

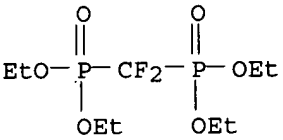
CN Phosphonic acid, (fluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



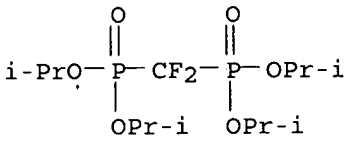
RN 78715-57-8 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



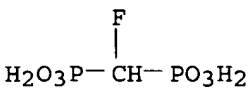
RN 78715-58-9 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetraethyl ester (9CI) (CA INDEX NAME)



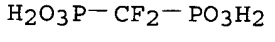
RN 78715-59-0 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



IT **10595-93-4P 10596-32-4P 78715-62-5P 78715-63-6P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 10595-93-4 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis- (9CI) (CA INDEX NAME)



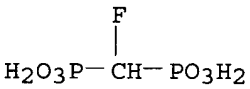
RN 10596-32-4 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis- (9CI) (CA INDEX NAME)



RN 78715-62-5 HCAPLUS
CN Phosphonic acid, (fluoromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

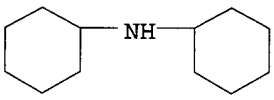
CM 1

CRN 10595-93-4
CMF C H5 F O6 P2



CM 2

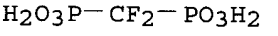
CRN 101-83-7
CMF C12 H23 N



RN 78715-63-6 HCAPLUS
CN Phosphonic acid, (difluoromethylene)bis-, compd. with N-cyclohexylcyclohexanamine (1:3) (9CI) (CA INDEX NAME)

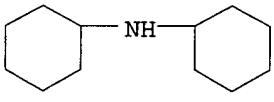
CM 1

CRN 10596-32-4
CMF C H4 F2 O6 P2



CM 2

CRN 101-83-7
CMF C12 H23 N



L17 ANSWER 25 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1980:123437 HCAPLUS
DOCUMENT NUMBER: 92:123437
TITLE: Diphosphonate herbicides
INVENTOR(S): Kuwabara, Masao; Mutsuto, Motoo; Matsunaga, Masashi; Iwazawa, Yoshihiro; Kawamura, Juji; Ooya, Tsunehiko; Igai, Takashi
PATENT ASSIGNEE(S): Nissan Chemical Industries, Ltd., Japan
SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.
CODEN: JKXXAF
DOCUMENT TYPE: Patent
LANGUAGE: Japanese
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

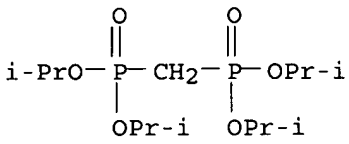
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 54147925	A2	19791119	JP 1978-55929	19780511

PRIORITY APPLN. INFO.: JP 1978-55929 A 19780511

AB Diphosphonates (HO)2P(:O)CXYP(:O)(OH)2 (X and Y = H, halo, alkyl, or cycloalkyl) are nonselective herbicides. Thus, (HO)2P(:O)CHEtP(:O)(OH)2 [4764-19-6] controlled Echinochloa crus-galli, Digitaria sanguinalis, Chenopodium ficifolium, Portulaca oleraceae, and Erigeron linifolius, but was phytotoxic to tomato, cucumber, and rice. Synthesis is given.

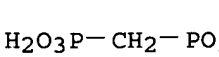
IT **1660-95-3**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(methylation and hydrolysis of)

RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)

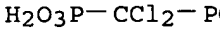


IT **1984-15-2P 10596-23-3P**
RL: AGR (Agricultural use); BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); **PREP (Preparation)**; USES (Uses)
(preparation and herbicidal activity of)

RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)



RN 10596-23-3 HCAPLUS
CN Phosphonic acid, (dichloromethylene)bis- (9CI) (CA INDEX NAME)



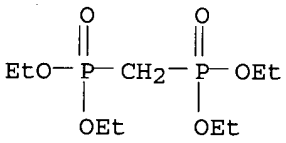
L17 ANSWER 26 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1979:104116 HCAPLUS
DOCUMENT NUMBER: 90:104116
TITLE: Phosphonic and phosphinic acids
INVENTOR(S): Thamm, Horst Dieter; Kleoner, Hans Jerg
PATENT ASSIGNEE(S): Hoechst A.-G., Fed. Rep. Ger.
SOURCE: Ger. Offen., 18 pp.
CODEN: GWXXBX
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 2719385	A1	19781102	DE 1977-2719385	19770430
DE 2719385	B2	19810730		
DE 2719385	C3	19820519		

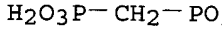
PRIORITY APPLN. INFO.: DE 1977-2719385 A 19770430

AB HO2C(CH2)nP(O)(OH)2 (n = 1, 2), (HO)2P(O)(CH2)nP(O)(OH)2 (n = 1, 4), Me(Cl3C)P(O)OH, HO2C(CH2)2P(O)(OH)Me, ClCH2P(O)(OH)2, and PhCH2CH2P(O)(OH)2 were prepared in 85-94% yields by transesterification of their Et and Me esters with HOAc. Thus, 0.5 mol EtO2CCH2P(O)(OEt)2 was transesterified with 2.25 mol HOAc in the presence of 0.024 mol H2SO4 to give 93% HO2CCH2P(O)(OH)2.

IT **1660-94-2**
RL: **RCT (Reactant)**; **RACT (Reactant or reagent)**
(hydrolysis of)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



IT **1984-15-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)

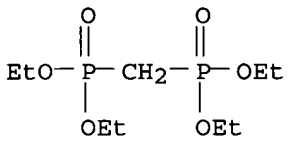


L17 ANSWER 27 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1975:25739 HCAPLUS
DOCUMENT NUMBER: 82:25739
TITLE: Organic polymeric polyphosphonates as potential preventive agents of dental caries. In vitro experiments
AUTHOR(S): Anbar, M.; St. John, G. A.; Scott, A. C.
CORPORATE SOURCE: Stanford Res. Inst., Menlo Park, CA, USA

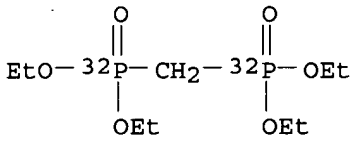
SOURCE: Journal of Dental Research (1974), 53(4), 867-78
CODEN: JDREAF; ISSN: 0022-0345
DOCUMENT TYPE: Journal
LANGUAGE: English

AB The anticariogenic effects of polyphosphonates were due to their adsorption on enamel surfaces as a monolayer. They inhibited Ca [7440-70-2] and F [16984-48-8] transport, but not that of phosphate. Adsorption of protein was diminished and adsorbed protein was readily desorbed from surfaces with polyphosphonates. Preparation of the polymers was described.

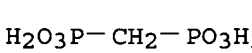
IT **1660-94-2P 53459-45-3P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and hydrolysis of)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



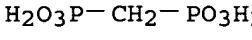
RN 53459-45-3 HCAPLUS
CN Phosphonic-32P acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



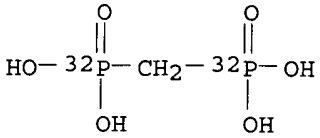
IT **1984-15-2P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation and tooth caries prevention by)
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)



IT **6145-29-5P 53459-46-4P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 6145-29-5 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrasodium salt (9CI) (CA INDEX NAME)

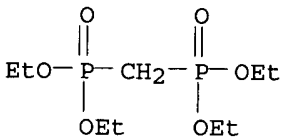


RN 53459-46-4 HCAPLUS
CN Phosphonic-32P acid, methylenebis-, tetrasodium salt (9CI) (CA INDEX NAME)

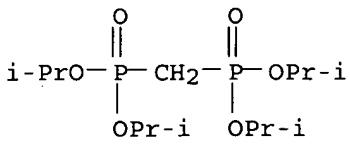


●4 Na

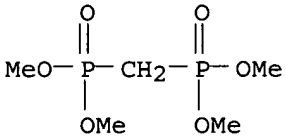
L17 ANSWER 28 OF 28 HCAPLUS COPYRIGHT 2005 ACS on STN
ACCESSION NUMBER: 1968:459337 HCAPLUS
DOCUMENT NUMBER: 69:59337
TITLE: Metalated methylenediphosphonate esters. Preparation, characterization and synthetic applications
AUTHOR(S): Quimby, O. T.; Curry, J. D.; Nicholson, D. Allan; Prentice, J. B.; Roy, C. H.
CORPORATE SOURCE: Miami Valley Lab., Procter and Gamble Co., Cincinnati, OH, USA
SOURCE: Journal of Organometallic Chemistry (1968), 13(1), 199-207
CODEN: JORCAI; ISSN: 0022-328X
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The metalation of esters of tetraalkyl methylenediphosphonates with Na, K, NaH, and BuLi to form the corresponding salts, M+[CH(PO3R2)2]-, is described. These compds. were characterized by 31P and 1H N.M.R.; their synthetic usefulness was demonstrated by the preparation of a variety of alkylates, R1CH(PO3R2)2, and by the preparation of mono and dihalo derivs., XCH(PO3R2)2 and X2C(PO3R2)2, by direct halogenation. A superior method of halogenation of tetraalkyl methylenediphosphonates is also described. The reaction of metalated tetraalkyl methylenediphosphonate with mol. O in toluene is shown to be complex.
IT **1660-94-2P 1660-95-3P 16001-93-7P**
RL: **RCT (Reactant)**; SPN (Synthetic preparation); PREP (Preparation); **RACT (Reactant or reagent)**
(preparation and metalation of)
RN 1660-94-2 HCAPLUS
CN Phosphonic acid, methylenebis-, tetraethyl ester (9CI) (CA INDEX NAME)



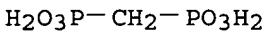
RN 1660-95-3 HCAPLUS
CN Phosphonic acid, methylenebis-, tetrakis(1-methylethyl) ester (9CI) (CA INDEX NAME)



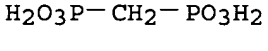
RN 16001-93-7 HCAPLUS
CN Phosphonic acid, methylenebis-, tetramethyl ester (9CI) (CA INDEX NAME)



IT **1984-15-2DP**, Phosphonic acid, methylenedi-, tetraalkyl esters, sodium complexes **1984-15-2P 21294-93-9P**
RL: SPN (Synthetic preparation); **PREP (Preparation)**
(preparation of)
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)



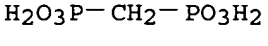
RN 1984-15-2 HCAPLUS
CN Phosphonic acid, methylenebis- (9CI) (CA INDEX NAME)



RN 21294-93-9 HCAPLUS
CN Phosphonic acid, methylenedi-, compd. with aniline (8CI) (CA INDEX NAME)

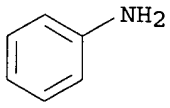
CM 1

CRN 1984-15-2
CMF C H6 O6 P2



CM 2

CRN 62-53-3
CMF C6 H7 N


NH2